Front cover: Historical remarks to the Institute for Chemical Research (ICR)

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The crystal structure shown on the front cover represents a ternary inclusion complex of a flavin coenzyme model compound which was synthesized in Ohno Laboratory.

In the laboratory, the reaction mechanism and stereochemistry of redox enzymes have been studied from the view point of physical organic chemistry. In 1992 the introduction of an X-ray diffractometer made it possible to investigate the structure of various coenzyme model compounds.

By comparing the geometry of a flavin coenzyme model compound which includes a hydrogen bond in a crystal with that of the same molecule which does not, it is possible to simulate geometrical change observed when an oxidized flavin coenzyme is activated through hydrogen bonding with apoproteins at the active site. In the series of the X-ray crystallographic analyses of these crystals, it has been confirmed that the included molecule brings a geometrical change of the flavin skeleton such as the lengths of conjugated bonds, N(1)-C(10a)-C(4a)-C(5), participating in redox reaction. The geometry of a flavin compound on the oxidized form are brought close to that of its reduced form through hydrogen bonding at the pyrimidine ring. This observation strongly supports the proposal that the geometry of an oxidized flavin coenzyme at the active site of the enzyme is distorted into an activated form through hydrogen bonding with the functional groups of apoproteins, which is considerably different from that undistorted.